

Variational Path Integral For Fermions: Calculations for Liquid ^3He

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Abstract

We present a study of the ground-state of liquid ^3He at zero pressure. We project the ground-state of the system from a Jastrow-Slater wave function using an implementation of the Variational Path Integral method. We have calculated the ground-state energy of the system and shown that this is a viable method to compute properties of fermionic systems.

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I. INTRODUCTION

The study of properties of liquid ^3He is of interest in its own right and also because, in the context of quantum Monte Carlo methods, it presents the so called sign problem due to the Fermi-Dirac statistics that this system must obey. In this work we address both these issues. A milestone in Monte Carlo calculations of quantum many-body systems is the investigation of the properties of liquid ^4He using the Variational Monte Carlo (VMC) method by McMillan in 1965¹. Not long after, variational calculations were extended by considering the solid phase of ^4He ². The fermionic system formed from ^3He atoms were addressed by Ceperley and collaborators³. Improved results were obtained by the introduction of triplet and backflow correlations in the trial wave function⁴ and also by new classes of trial wave functions⁵⁻⁸. Since then, the variational Monte Carlo method have also been applied in the study of many other systems. In addition, exact quantum Monte Carlo methods were implemented, such as Green's Function Monte Carlo⁹, Diffusion Monte Carlo (DMC)^{10,11} and Variational Path Integral (VPI)¹² methods which are able to calculate the exact value of the ground-state energy of bosonic systems or an upper bound for fermionic systems compatible with a given guiding function within only statistical uncertainties.

Typically, the Monte Carlo methods that computes properties of the exact ground-state of the system presents a sign problem when applied to study fermionic systems. This problem arises from the fact that a fermionic wave function can be negative. Techniques as the fixed-node (FN)¹¹ or released-node (RN)¹³ can be used together with the DMC method to obtain an upper bound value or an exact ground-state energy of a fermionic system. The FN approximation consist in restricting the movement of particles during the simulation to regions where the guiding function does not change sign. As far as we know, no one has applied the VPI method to calculate properties of a fermionic system. This method was introduced by Ceperley¹² by the name of VPI, latter it was also used by Sarsa *et al.*¹⁴ with the name of Path Integral Ground State (PIGS) method. In both these cases it was applied to study a system formed from the bosonic isotope of helium with results in excellent agreement with experimental data. In this work we aim to extend the method to fermionic systems, and calculate the ground-state energy of liquid ^3He . This method has some advantages over other quantum Monte Carlo calculations, the first one is its similarity with the variational method where the calculations are very straightforward. However unlike the variational

method, the VPI provides exact estimations for bosonic systems. A second advantage is the calculation of expected values of any operator without any extrapolation, an approximation one must follow in the DMC method for calculations of quantities associated to operators that do not commute with the Hamiltonian. And finally, for fermionic systems, it provides us a very simple manner to deal with the fermionic sign problem through the fixed node approximation. In the next section we give a review of the VPI method as it was first proposed and we explain how we extended it for a fermionic system.

II. METHODS

The system we consider is composed by N atoms of ^3He inside a three dimensional cubic box with periodic boundary conditions applied on each face. The atoms interact with each other via the HFD-B3-FC11 pairwise potential proposed by Aziz and coworkers¹⁵. We assume that the atoms are equally distributed between the two spin states (up and down) and that there is no external potential involved, therefore the Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{2m} \sum_{i=1}^N \mathbf{p}_i^2 + \sum_{i<j}^N v(|\mathbf{r}_i - \mathbf{r}_j|), \quad (1)$$

where m is the helium mass, \mathbf{p}_i and \mathbf{r}_i are the momentum and the coordinates of the i -th atom, and $v(r)$ is the inter-atomic potential.

If to a trial state $|\Psi_T\rangle$ describing this system we apply the projector $\rho(\beta) = e^{-\beta\mathcal{H}}$ the new state $|\phi(\beta)\rangle = \rho(\beta) |\Psi_T\rangle$ will satisfy

$$\lim_{\beta \rightarrow \infty} |\phi(\beta)\rangle \propto |\phi_0\rangle, \quad (2)$$

if $|\Psi_T\rangle$ has an overlap with the ground-state $|\phi_0\rangle$ of \mathcal{H} . The projector $\rho(\beta)$ is formally equal to the density matrix operator of the canonical ensemble where β is the inverse of the temperature. Another interpretation of $\rho(\beta)$ is the time evolution operator with β being the imaginary time.

We now define the average energy

$$E(\beta) = \frac{\langle \phi(\beta) | \mathcal{H} | \phi(\beta) \rangle}{\langle \phi(\beta) | \phi(\beta) \rangle}, \quad (3)$$

and see that, as β increases, $E(\beta)$ decreases exponentially creating a sequence of upper bound values for the ground-state energy E_0 . This sequence asymptotically converges to E_0 . For the calculation of $E(\beta)$ we use the propagator $\rho(\beta)$ in the representation of the coordinate space. For this purpose we need an expression for the matrix element $\rho(R, R', \beta) = \langle R | \rho(\beta) | R' \rangle$, where $R = \{\mathbf{r}_i : i = 1, 2, \dots, N\}$ is the configuration of the N atoms system. The exact expression for $\rho(R, R', \beta)$ is given by the Feynman-Kac formula¹² and involves an integral over all paths $R(t)$ connecting $R(t = 0) = R$ and $R(t = \beta) = R'$ within an imaginary time β . The evaluation of this path integral can be performed by dividing β into M “time” slices $\tau = \beta/M$ and by the integration over the intermediate configurations $R(t = n\tau) = R_n$, $n = 1, 2, \dots, M - 1$, thus we have

$$\rho(R, R', \beta) = \int dR_1 \dots dR_{M-1} \rho(R, R_1, \tau) \rho(R_1, R_2, \tau) \dots \rho(R_{M-1}, R', \tau). \quad (4)$$

It is easy to see that Eq.(4) is exact if $\rho(R_n, R_{n+1}, \tau)$ also is, but again we would have to deal with the path integral that we are trying to avoid. There are some approximated expressions for $\rho(R, R', \tau)$ that when τ is small enough have errors lower than the statistical uncertainty of a Monte Carlo simulation. In this paper we have used the simple primitive approximation

$$\rho(R_n, R_{n+1}, \tau) \approx (4\pi\lambda\tau)^{-\frac{3N}{2}} e^{-\frac{(R_{n+1}-R_n)^2}{4\lambda\tau} - \tau \frac{[V(R_{n+1})+V(R_n)]}{2}}, \quad (5)$$

where $\lambda = \hbar^2/2m$ and

$$V(R) = \sum_{i < j} v(|\mathbf{r}_i - \mathbf{r}_j|). \quad (6)$$

Until now we did not have taken into consideration the statistic obeyed by the atoms in the system, as a matter of fact, the density matrix given by Eqs. (4) and (5) respect the statistic of a system of distinguishable particles. Our system is formed from indistinguishable fermionic atoms, and the projector, our density matrix, should be antisymmetric under permutation of atomic coordinates. In the VPI method we do not need to be concerned with these permutations in $\rho(R, R', \beta)$ as long as we choose a trial wave function with the proper symmetry. We shall prove this assumption, in general, for a fermionic many-body system. Let $\rho_F(R, R', \beta)$ be a matrix element of a fermionic density matrix,

$$\rho_F(R, R', \beta) = \frac{1}{N!} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} \rho(\mathcal{P}R, R', \beta) \quad (7)$$

with $\rho(R, R', \beta)$ given by Eqs.(4) and (5), and $\mathcal{P}R$ a permutation of R with \mathcal{P} exchanges of atomic coordinates. Therefore we can rewrite Eq.(3) as

$$E(\beta) = \frac{1}{N!} \sum_{\mathcal{P}} \int dR_1 dR_2 \dots dR_{2M+1} (-1)^{\mathcal{P}} P(\mathcal{P}, R_1, R_2, \dots, R_{2M+1}) E_L(R_{2M+1}), \quad (8)$$

where $E_L(R) = \mathcal{H}_R \Psi_T(R) / \Psi_T(R)$, \mathcal{H}_R is the coordinate representation of the Hamiltonian, and

$$P(\mathcal{P}, R_1, R_2, \dots, R_{2M+1}) = \frac{\Psi_T(R_1) \rho(\mathcal{P}R_1, R_2, \tau) \dots \rho(R_{2M}, R_{2M+1}, \tau) \Psi_T(R_{2M+1})}{\langle \phi(\beta) | \phi(\beta) \rangle}. \quad (9)$$

To reach the expression of Eq.(8) we use the fact that \mathcal{H} commutes with $\rho(\beta)$ and then $\langle \Psi_T | \rho(\beta) \mathcal{H} \rho(\beta) | \Psi_T \rangle = \langle \Psi_T | \rho(\beta) \rho(\beta) \mathcal{H} | \Psi_T \rangle$. It is important to notice that the permutation is not made in $\Psi_T(R_1)$, and since the trial function is antisymmetric we can replace $(-1)^{\mathcal{P}} \Psi_T(R_1)$ by $\Psi_T(\mathcal{P}R_1)$ in Eqs.(8) and (9). Thus, the integration over all the $N!$ permutations give the same contribution to the energy and therefore we do not need to be concerned with the permutations. It is worth mentioning that it is possible to extend this method to calculate averages of operators that do not commute with $\rho(\beta)$, and the expression for the expected value of this operator is very similar to Eq.(8).

We need now to choose a trial wave function $\Psi_T(R)$ that respects the statistic of the fermionic system, $\Psi_T(R)$ has to be antisymmetric under exchange of atomic coordinates. But, for an antisymmetric trial wave function the product $\Psi_T(R_1) \Psi_T(R_{2M+1})$ in Eq.(9) could be negative which gives rise to a sign problem in the VPI method. However, to avoid this problem we only need to restrict the integration to regions where $\Psi_T(R_1) \Psi_T(R_{2M+1})$ does not change sign.

In this paper we chose the well known Jastrow-Slater wave function³ as the trial wave function to perform the VPI calculation in a system formed from ^3He atoms,

$$\Psi_T(R) = D(R) \prod_{i < j} e^{-\frac{1}{2} u(|\mathbf{r}_i - \mathbf{r}_j|)}, \quad (10)$$

where $u(r) = (b/r)^5$ and $D(R)$ is a product of two Slater determinants, one for the spin up atoms and the other for the spin down atoms. We chose plane waves as the one-body states of $D(R)$.

The integration of Eq.(8) is $3N(2M + 1)$ -dimensional with an effective configuration given by $(R_1, R_2, \dots, R_{2M+1})$. The value of this integral can be estimated by the Monte Carlo method. Configurations R_1 and R_{2M+1} associated with the path's ends are drawn by the standard Metropolis algorithm with the constraint $\Psi_T(R_1)\Psi_T(R_{2M+1}) > 0$. The configurations associated with beads R_i , $2 \leq i \leq 2M$, were sampled by a multi-level Metropolis bisection algorithm. The sampling with L levels is performed as follows. We randomly select a fragment of $2^L + 1$ contiguous beads, here we can include the end of the path as well, since the ends of the fragment remain fixed. In the first level we bisect the path fragment in the middle, and the configuration of this particular bead is sampled and eventually accepted with the Metropolis criterion. In the second level, we bisect the two half fragments originated from the first level and sample new coordinates for the beads in the middle of each half fragment. We keep doing this bisection and sample process until all L levels were considered or a proposed configuration is rejected. In this case the simulation proceeds from the unchanged path. In other words, a new path is accepted only if all sampled configurations have been accepted. More details from this bisection algorithm are given in reference¹².

With the aim of estimating the ground-state energy E_0 of the liquid phase of the system, we fix the “time” slice τ and increase its number M , obtaining a sequence of energies $E(\beta = M\tau)$. For M large enough this sequence converges to a minimum that is compatible with the nodal structure of the chosen $\Psi_T(R)$.

III. RESULTS

The ground-state energy of liquid ^3He was computed at equilibrium density $\rho_0 = 0.0163 \text{ \AA}^{-3}$. We applied the VPI method in a system of $N = 54$ atoms with periodic boundary conditions. As we have mentioned in Sec. II, we use a Jastrow-Slater wave function as a trial function at the ends of the path. This wave function is the one of Eq.(10), it depends on the parameter b which is chosen by the minimization of the variational energy.

In our calculations we have used $b = 2.89 \text{ \AA}$ which gives a variational energy of $-1.14 \pm 0.03 \text{ K/atom}$.

We project the ground-state from this trial wave function using the density matrix $\rho(\beta)$. The total “time” β is divided into M slices τ . For τ fixed and by increasing M we can asymptotically reach the ground-state. In coordinate representation this method creates a path of $2M + 1$ beads, those that are not at the ends of the path are moved by a multi-level Metropolis algorithm. For small values of M we have used a Metropolis of level $L = 1$ with $\tau = 0.001 \text{ K}^{-1}$, and for large values we have used $L = 3$ with $\tau = 0.0005 \text{ K}^{-1}$. We have calculated the energy $E(\beta)$ given by Eq.(8) and the results are shown in Table I and plotted in Fig.1. In the figure $E(\beta = 0)$ stands for the variational energy.

The results show that energies with the same value of β but different values of L (τ and M) are equivalent within the statistical uncertainty. Moreover we can also see that the energy converges to a minimum. In Fig. 1 we can see the approximate exponential decay of the upper bound energies $E(\beta)$ to its minimum. This value is in excellent agreement with values from the literature¹⁶ obtained using other possibly more laborious methods. For the three largest values of the time slices M , after equilibration, 2.4×10^6 steps were considered to estimate the energies. As the number of time slices M decreased equilibration was reached more quickly and less steps were required for the statistical uncertainties reported.

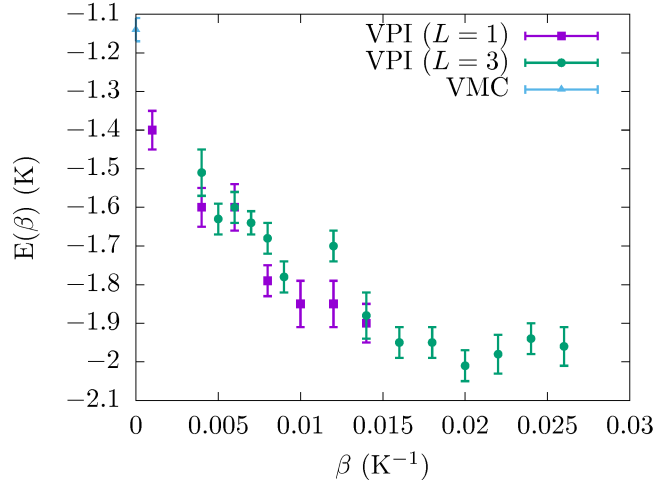


FIG. 1. Upper bound energies $E(\beta)$. Squares (purple) represent the VPI calculations with $L = 1$, circles (green) stand for VPI calculations with $L = 3$ and the triangle (blue) represents the VMC result.

TABLE I. Energy $E(\beta)$ with $\beta = M\tau$, L is the level of the multi-level Metropolis sampling algorithm. For $L = 1$ we have used $\tau = 1 \times 10^{-3} \text{ K}^{-1}$ and for $L = 3$, $\tau = 5 \times 10^{-4} \text{ K}^{-1}$.

$\beta \text{ (K}^{-1}\text{)}$	$E(\beta) \text{ (K/atom)}$	$E(\beta) \text{ (K/atom)}$
	$L = 1$	$L = 3$
0.001	-1.40 ± 0.05	—
0.004	-1.60 ± 0.05	-1.51 ± 0.06
0.005	—	-1.63 ± 0.04
0.006	-1.60 ± 0.006	-1.60 ± 0.04
0.007	—	-1.64 ± 0.04
0.008	-1.79 ± 0.04	-1.68 ± 0.04
0.009	—	-1.78 ± 0.04
0.01	-1.85 ± 0.04	—
0.012	-1.85 ± 0.06	-1.70 ± 0.04
0.014	-1.90 ± 0.05	-1.88 ± 0.06
0.016	—	-1.95 ± 0.04
0.018	—	-1.95 ± 0.04
0.02	—	-2.01 ± 0.04
0.022	—	-1.98 ± 0.05
0.024	—	-1.94 ± 0.04
0.026	—	-1.96 ± 0.05

IV. CONCLUSIONS

We have shown that the Variational Path Integral method is a viable method to calculate the ground-state energy of a fermionic system made of ^3He atoms. We have used path with ends formed from the well known Jastrow-Slater wave function and projected out the ground-state. In fact, due to the well known poor nodal structure of the adopted wave function, we obtain an upper bound to the ground-state energy not so close to the experimental value at the equilibrium density, -2.47 K/atom . As a further work we want to introduce Feynman-Cohen backflow correlations to improve the nodal structure of the wave function to obtain values more close to experiment. Moreover and more important we want to compute

properties associated with operators that do not commute with the Hamiltonian. In this way, without the need of extrapolations that might add bias to the results, we want to see how the computed values compare with experiment.

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